



wwPDB EM Validation Summary Report ⓘ

Mar 6, 2026 – 02:24 PM UTC

PDB ID : 6SL1 / pdb_00006sl1
EMDB ID : EMD-10234
Title : Structure of the open conformation of CtTel1
Authors : Jansma, M.; Eustermann, S.E.; Kostrewa, D.; Lammens, K.; Hopfner, K.P.
Deposited on : 2019-08-16
Resolution : 3.60 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

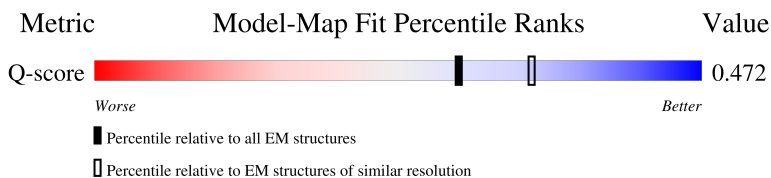
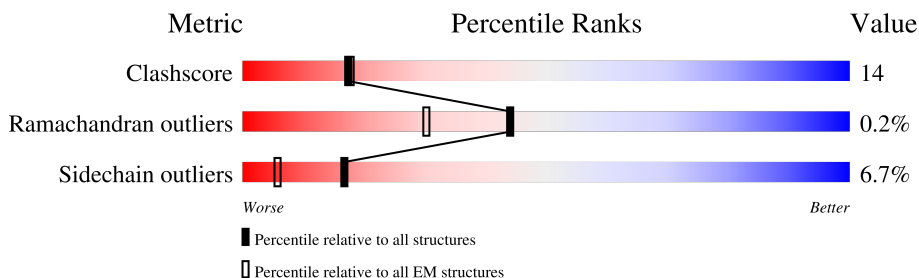
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12797 (3.10 - 4.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	2944	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 21041 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

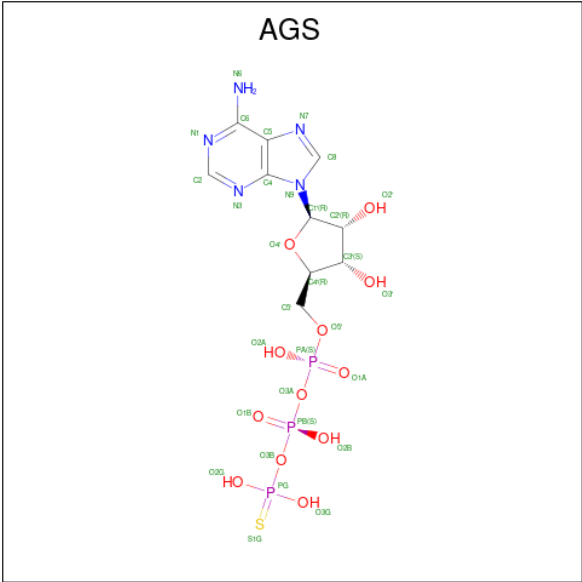
- Molecule 1 is a protein called Serine/threonine-protein kinase Tel1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2652	Total	C	N	O	S	0	0
			21009	13361	3665	3888	95		

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1489	SER	GLU	conflict	UNP G0S4S9
A	2847	LEU	PHE	conflict	UNP G0S4S9
A	2848	TYR	-	insertion	UNP G0S4S9
A	2849	GLN	-	insertion	UNP G0S4S9
A	2850	TRP	-	insertion	UNP G0S4S9
A	2851	SER	-	insertion	UNP G0S4S9
A	2852	ILE	-	insertion	UNP G0S4S9
A	2853	SER	-	insertion	UNP G0S4S9
A	2854	PRO	-	insertion	UNP G0S4S9
A	2855	VAL	-	insertion	UNP G0S4S9
A	2856	ARG	-	insertion	UNP G0S4S9
A	2857	MET	-	insertion	UNP G0S4S9
A	2858	ALA	-	insertion	UNP G0S4S9
A	2859	LYS	-	insertion	UNP G0S4S9
A	2860	LEU	-	insertion	UNP G0S4S9
A	2861	GLN	-	insertion	UNP G0S4S9
A	2862	ASN	-	insertion	UNP G0S4S9
A	2863	ALA	-	insertion	UNP G0S4S9
A	2864	ARG	-	insertion	UNP G0S4S9
A	2865	GLU	-	insertion	UNP G0S4S9
A	2866	VAL	-	insertion	UNP G0S4S9

- Molecule 2 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S).



Mol	Chain	Residues	Atoms						AltConf
			Total	C	N	O	P	S	
2	A	1	31	10	5	12	3	1	0

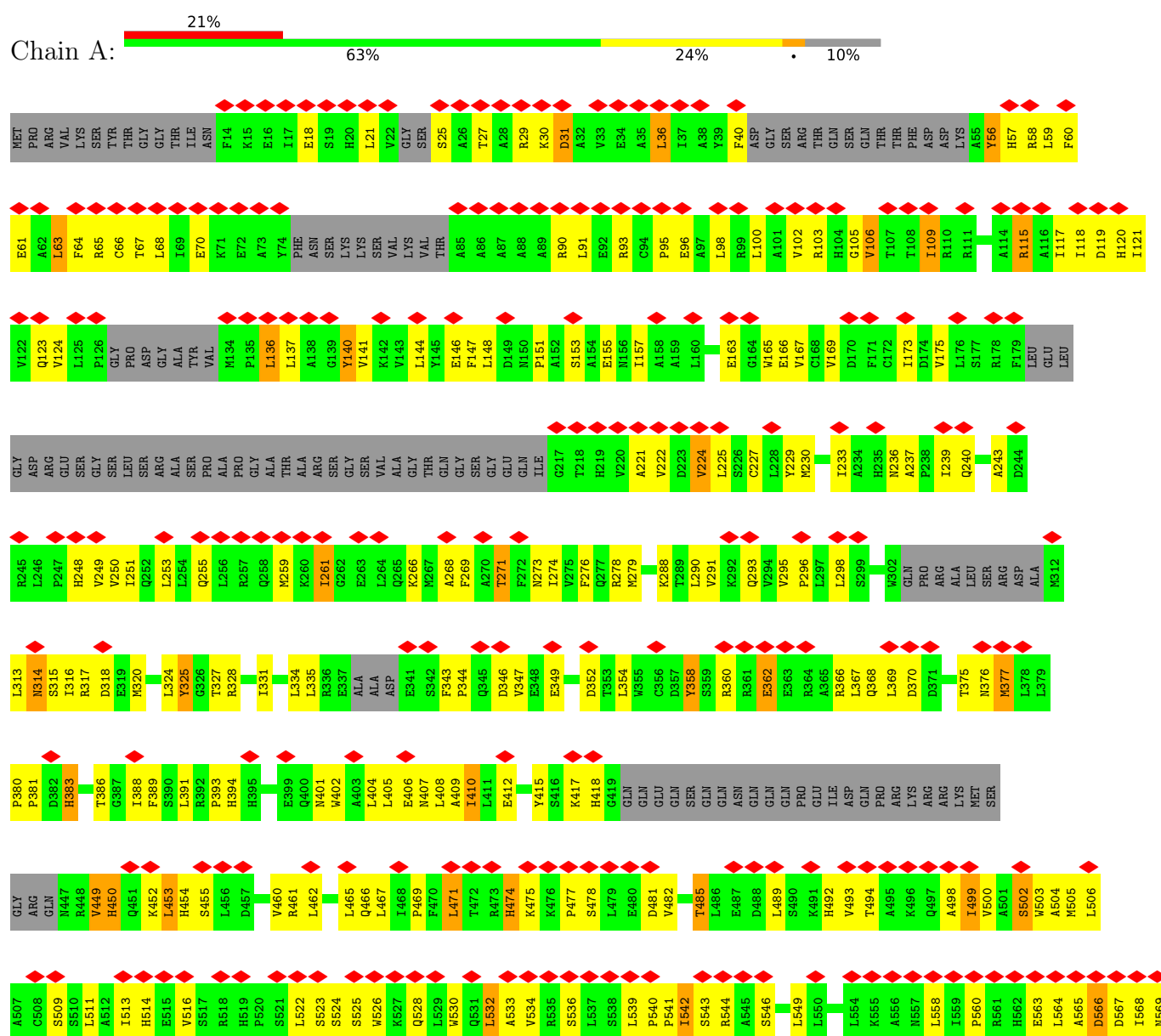
- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Mg	0
			1	1	

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Serine/threonine-protein kinase Tel1





GLU	ASP	GLY	GLU	GLY	GLY	VAL	LYS	LYS	LYS	GLU	LYS	GLN	ARG	PRO	ALA	ASN	GLU	PRO	S2897	E2898	A2899	D2900	R2901	A2902	I2903	V2916	D2922	Q2926	A2941	A2944																				
E2727	E2734	W2735	K2738	R2739	T2745	A2748	L2752	L2768	D2769	T2772	G2773	E2774	V2775	V2792	R2799	D2803	L2825	R2829	E2830	E2831	R2843	L2847	I2852	S2853	P2854	W2857	Q2861	N2862	ALA	ARG	GLU	VAL	GLY	GLY	GLY	VAL	GLY	GLY	GLY											
L2568	D2569	H2572	F2579	E2582	A2586	S2587	G2588	V2589	S2590	A2591	P2592	K2593	L2594	L2595	T2600	D2601	K2606	Q2607	L2608	G2612	N2613	D2614	D2615	L2616	E2631	K2634	L2635	H2636	R2647	T2648	Y2649	T2655	S2656	S2657	S2658	G2659	L2660	F2663	L2670	L2674	Y2681	F2725	H2726							
Q2471	A2472	R2473	T2474	R2475	V2476	N2477	K2478	D2479	D2480	E2481	V2482	A2483	V2484	S2485	R2486	Q2487	R2488	A2489	T2490	S2498	V2503	L2506	W2507	I2510	T2513	S2514	W2522	D2523	R2524	D2525	P2526	T2527	K2530	S2531	G2532	Q2533	P2536	I2537	P2541	L2547	W2550	N2553	P2557	P2558	N2567					
ALA	LYS	ASP	SER	GLN	LEU	ARG	ASN	ARG	TYR	GLN	S2347	H2348	L2349	A2350	K2351	A2352	K2353	Q2354	W2355	Q2356	E2357	L2358	Q2359	Q2360	Q2361	E2362	L2363	R2364	R2365	K2375	L2376	N2380	M2399	E2407	E2408	E2409	V2410	E2413	V2414	Q2439	D2440	H2441	T2442	L2443	L2444	F2445	Q2446	P2461	M2465	T2470
L2188	C2195	D2203	A2204	M2208	H2217	I2221	R2225	D2233	S2234	S2235	L2236	K2237	K2238	Q2239	S2244	D2247	K2282	E2287	D2307	E2310	D2311	L2312	A2313	R2314	L2315	Q2316	N2317	L2318	K2319	K2320	G2321	K2322	D2323	E2324	E2325	V2326	A2327	Q2328	L2329	K2330	ALA	LEU	ILE	ALA	SER					
S2045	E2051	L2052	D2053	L2063	K2064	V2067	R2068	H2069	G2073	S2074	T2077	L2080	L2084	G2085	A2086	L2087	A2088	T2091	E2092	R2100	D2101	T2108	L2109	F2111	T2112	E2113	K2114	R2115	S2116	K2117	W2118	R2123	D2126	D2136	L2159	L2162	R2163	G2164	W2165	I2171	L2182									
W1730	D1731	P1732	Y1733	P1736	L1737	S1738	D1739	GLN	PHE	S1914	I1915	I1916	E1919	N1923	I1924	D1925	D1936	L1943	N1950	D1951	G1952	F1958	R1959	D1964	D1971	L1972	P1799	H1803	L1804	Y1808	D1811	E1833	P1834	A1835	I1860	E1892	S1897	T1898	R1899	GLY	SER	ARG								
E1607	K1611	W1617	Q1623	R1624	G1634	G1638	R1639	S1640	F1641	A1642	V1647	P1648	E1649	D1650	L1651	L1652	R1653	E1654	Q1658	E1659	Y1660	R1661	Q1665	G1666	V1667	G1668	S1669	S1670	K1679	S1684	G1685	D1686	C1687	F1688	E1694	R1698	M1708	D1709	H1710	L1713	Q1717	S1728	N1729							

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	111910	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	55.5	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.068	Depositor
Minimum map value	-0.042	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0118	Depositor
Map size (Å)	372.768, 372.768, 372.768	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.059, 1.059, 1.059	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, AGS

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.45	0/21421	0.45	1/29018 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	1378	PRO	CA-N-CD	-9.24	99.07	112.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2481	GLU	Peptide
1	A	259	MET	Peptide
1	A	474	HIS	Peptide
1	A	677	MET	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	21009	0	21193	571	0
2	A	31	0	12	3	0
3	A	1	0	0	0	0
All	All	21041	0	21205	574	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

The worst 5 of 574 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1378:PRO:HD2	1:A:1379:GLU:H	1.20	1.06
1:A:1730:TRP:HZ3	1:A:1736:PRO:HD2	1.30	0.97
1:A:1730:TRP:CZ3	1:A:1736:PRO:HD2	2.00	0.96
1:A:2647:ARG:NH2	1:A:2774:GLU:OE2	2.06	0.88
1:A:2608:LEU:HD11	1:A:2663:PHE:HD1	1.40	0.86

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	2612/2944 (89%)	2388 (91%)	220 (8%)	4 (0%)	43 72

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2482	VAL
1	A	2483	ALA

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Mol	Chain	Res	Type
1	A	418	HIS
1	A	1377	GLU

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	2291/2529 (91%)	2137 (93%)	154 (7%)	15	42

5 of 154 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1185	LEU
1	A	2045	SER
1	A	1210	ILE
1	A	1313	ILE
1	A	2613	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 64 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2678	HIS
1	A	2770	HIS
1	A	1354	GLN
1	A	1345	HIS
1	A	2849	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	AGS	A	3001	3	32,33,33	0.90	4 (12%)	45,52,52	0.85	1 (2%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	AGS	A	3001	3	-	7/21/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	3001	AGS	PB-O3B	-2.94	1.56	1.59
2	A	3001	AGS	PB-O3A	-2.31	1.57	1.59
2	A	3001	AGS	PA-O3A	-2.03	1.57	1.59
2	A	3001	AGS	PG-S1G	2.02	1.95	1.90

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	3001	AGS	PB-O3B-PG	-4.83	115.48	133.17

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

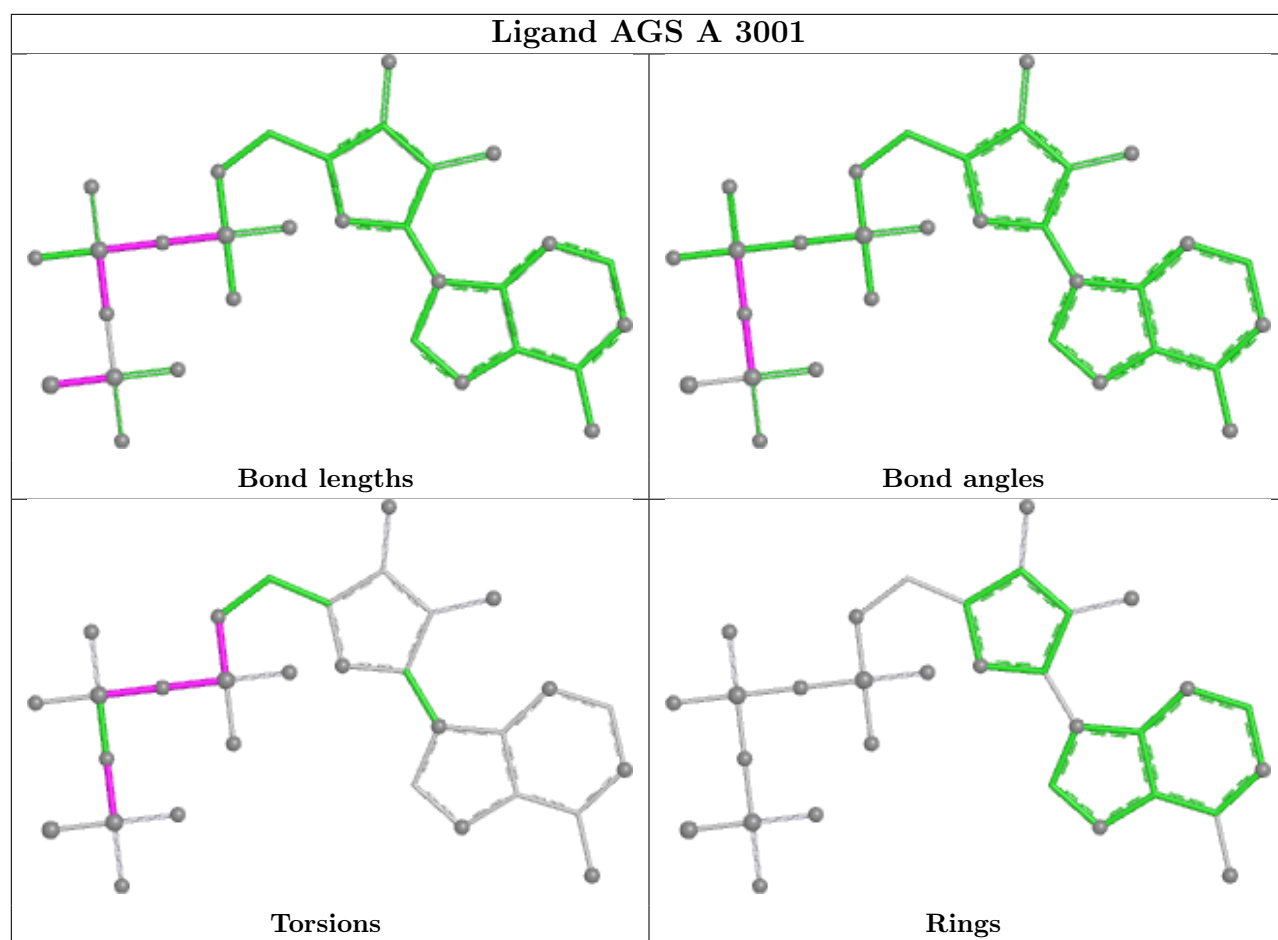
Mol	Chain	Res	Type	Atoms
2	A	3001	AGS	PB-O3B-PG-O2G
2	A	3001	AGS	PB-O3B-PG-O3G
2	A	3001	AGS	C5'-O5'-PA-O3A
2	A	3001	AGS	PB-O3A-PA-O5'
2	A	3001	AGS	C5'-O5'-PA-O1A

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	3001	AGS	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

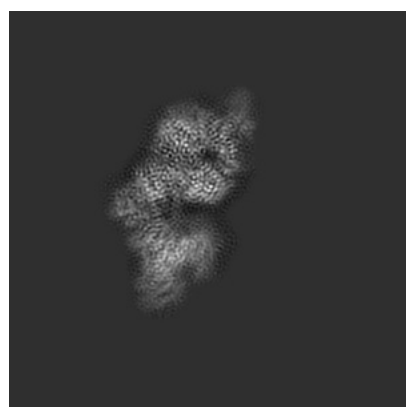
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10234. These allow visual inspection of the internal detail of the map and identification of artifacts.

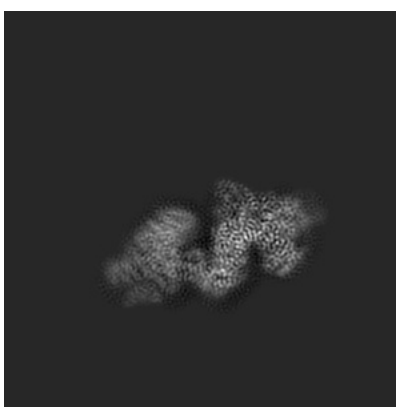
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

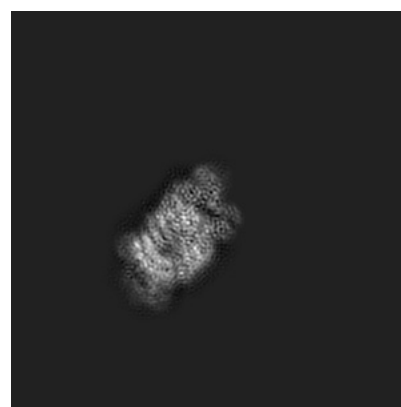
6.1.1 Primary map



X



Y

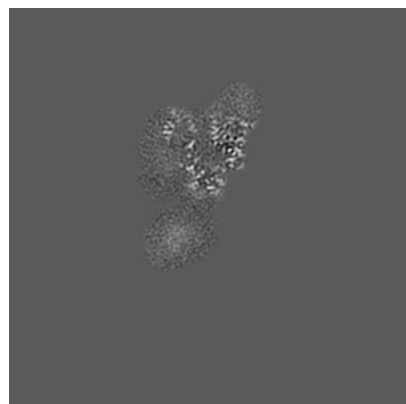


Z

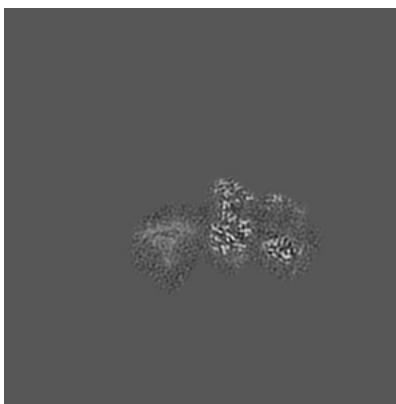
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

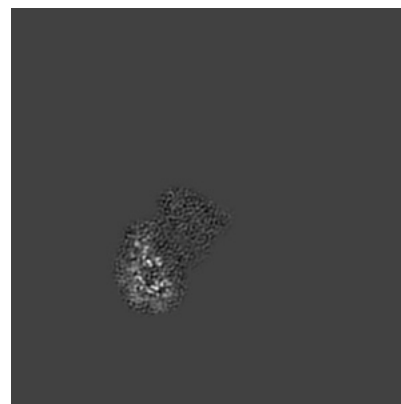
6.2.1 Primary map



X Index: 176



Y Index: 176

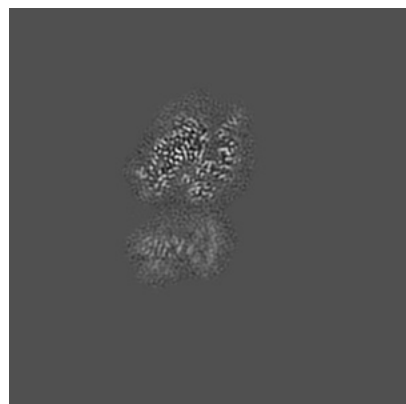


Z Index: 176

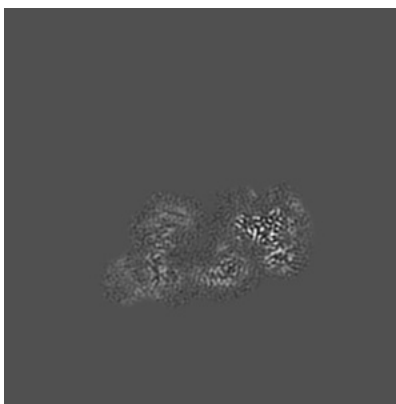
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

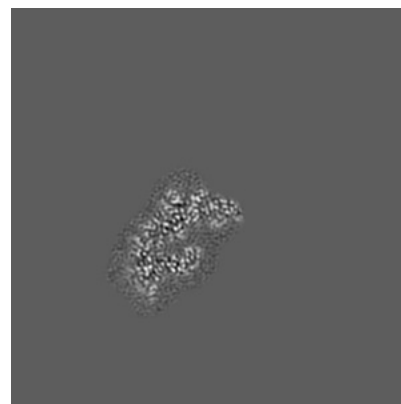
6.3.1 Primary map



X Index: 156



Y Index: 147

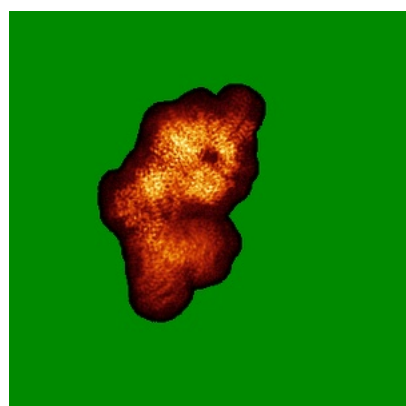


Z Index: 194

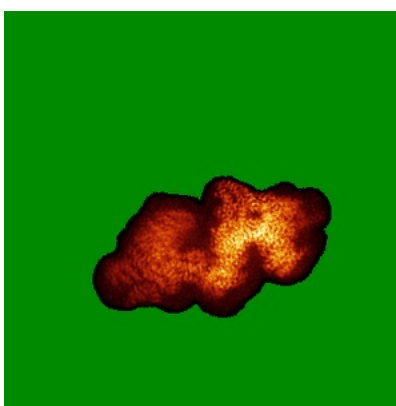
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

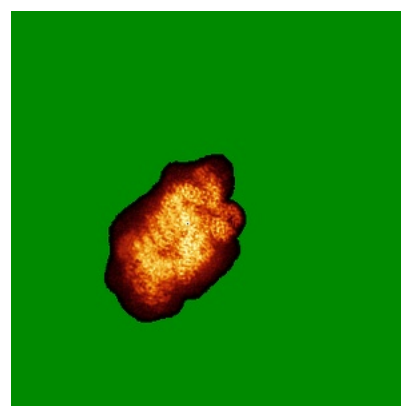
6.4.1 Primary map



X



Y

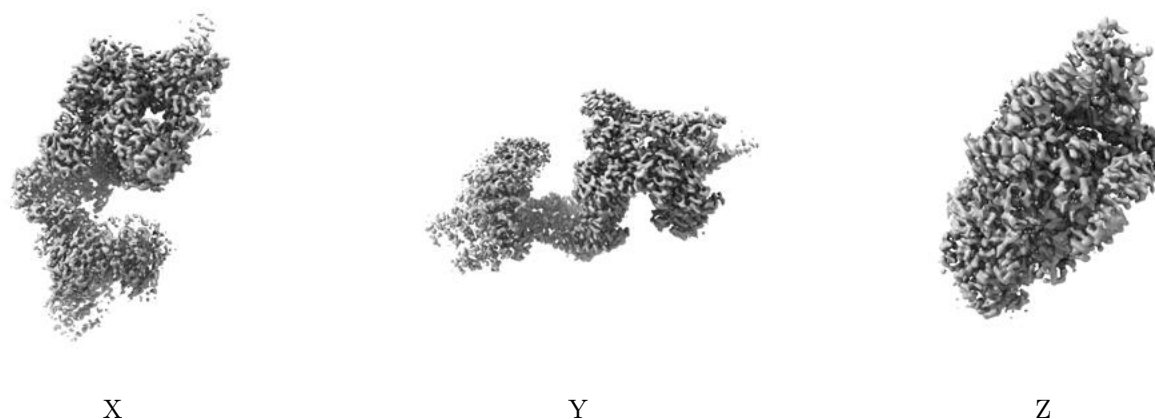


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0118. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

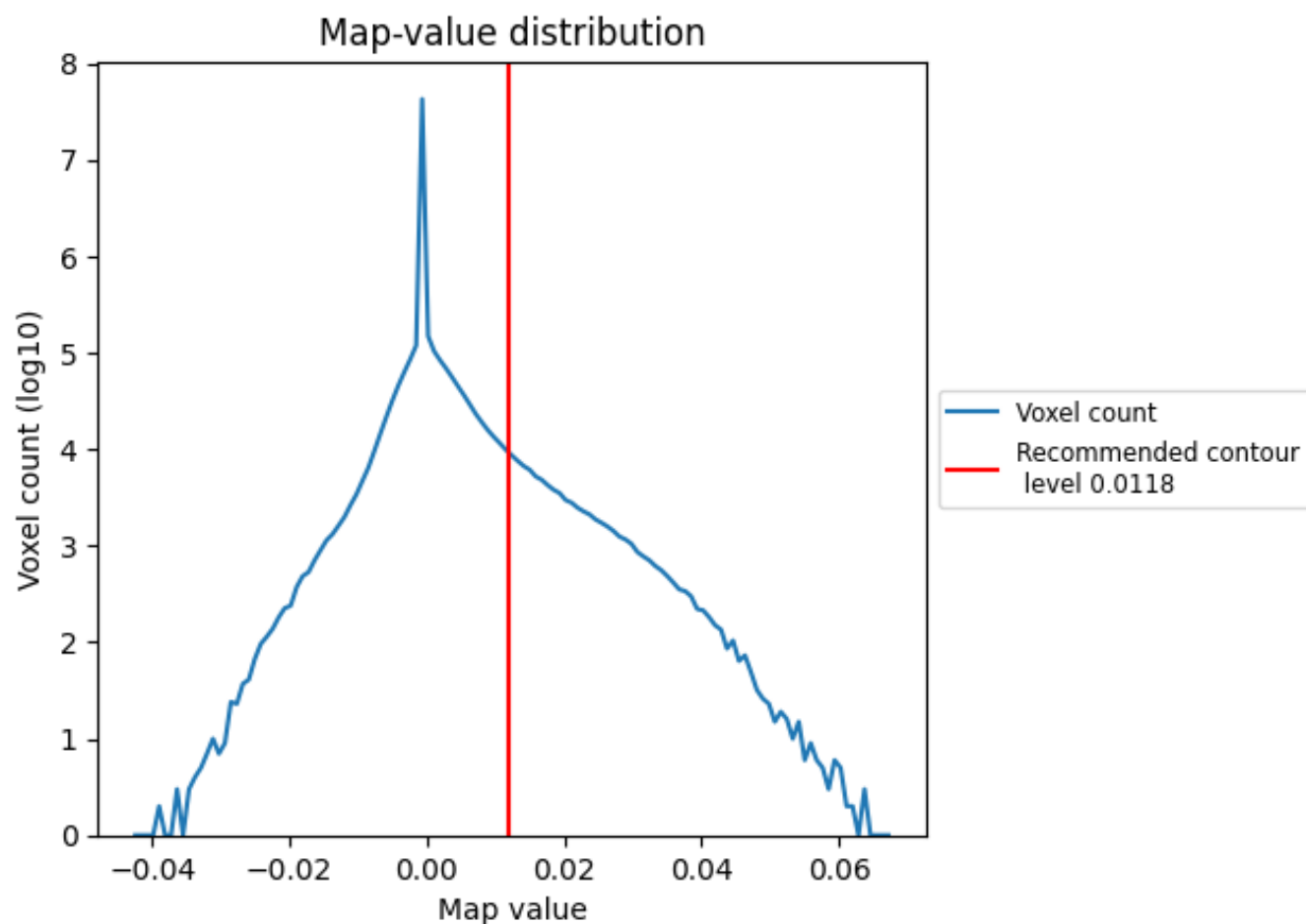
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

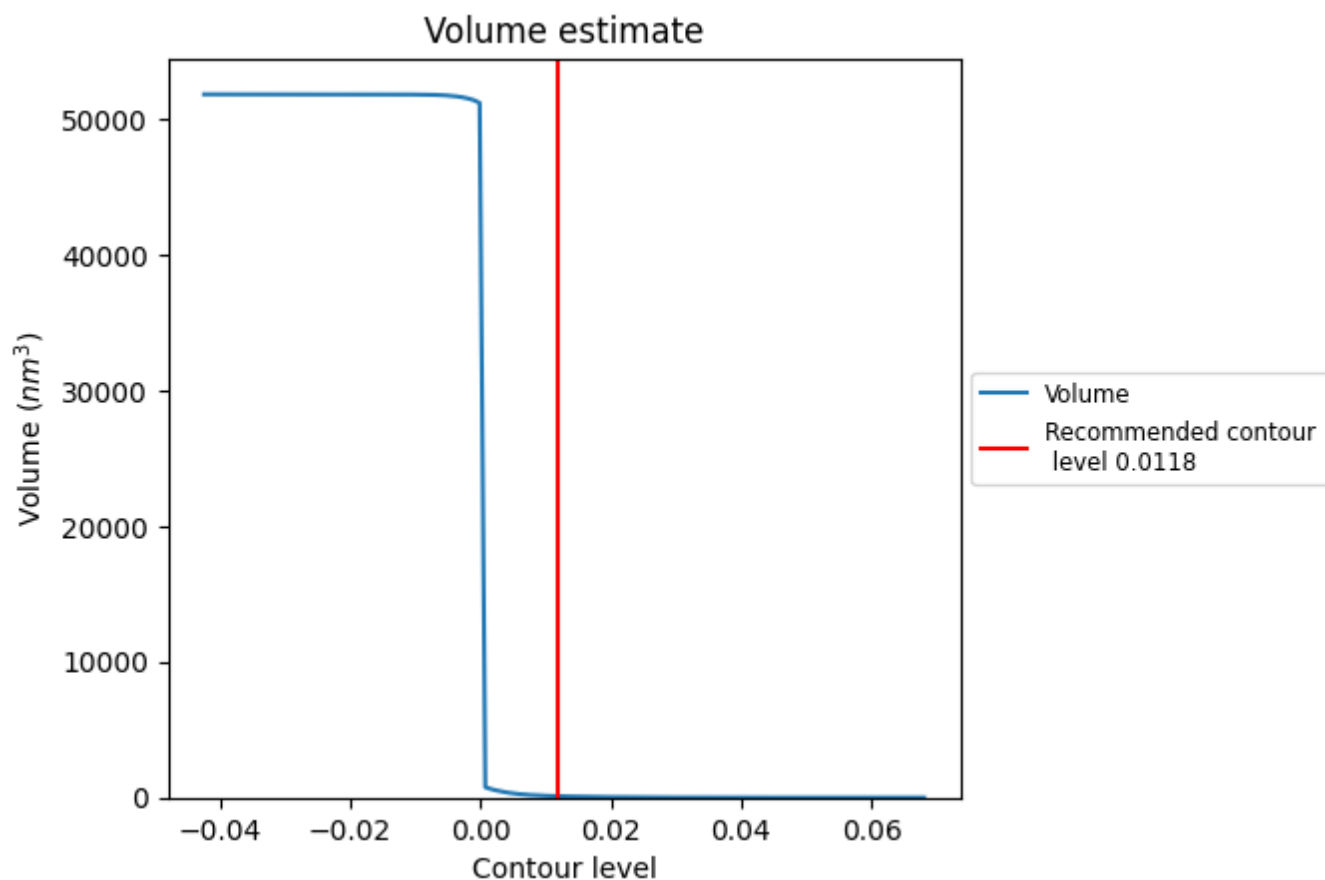
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

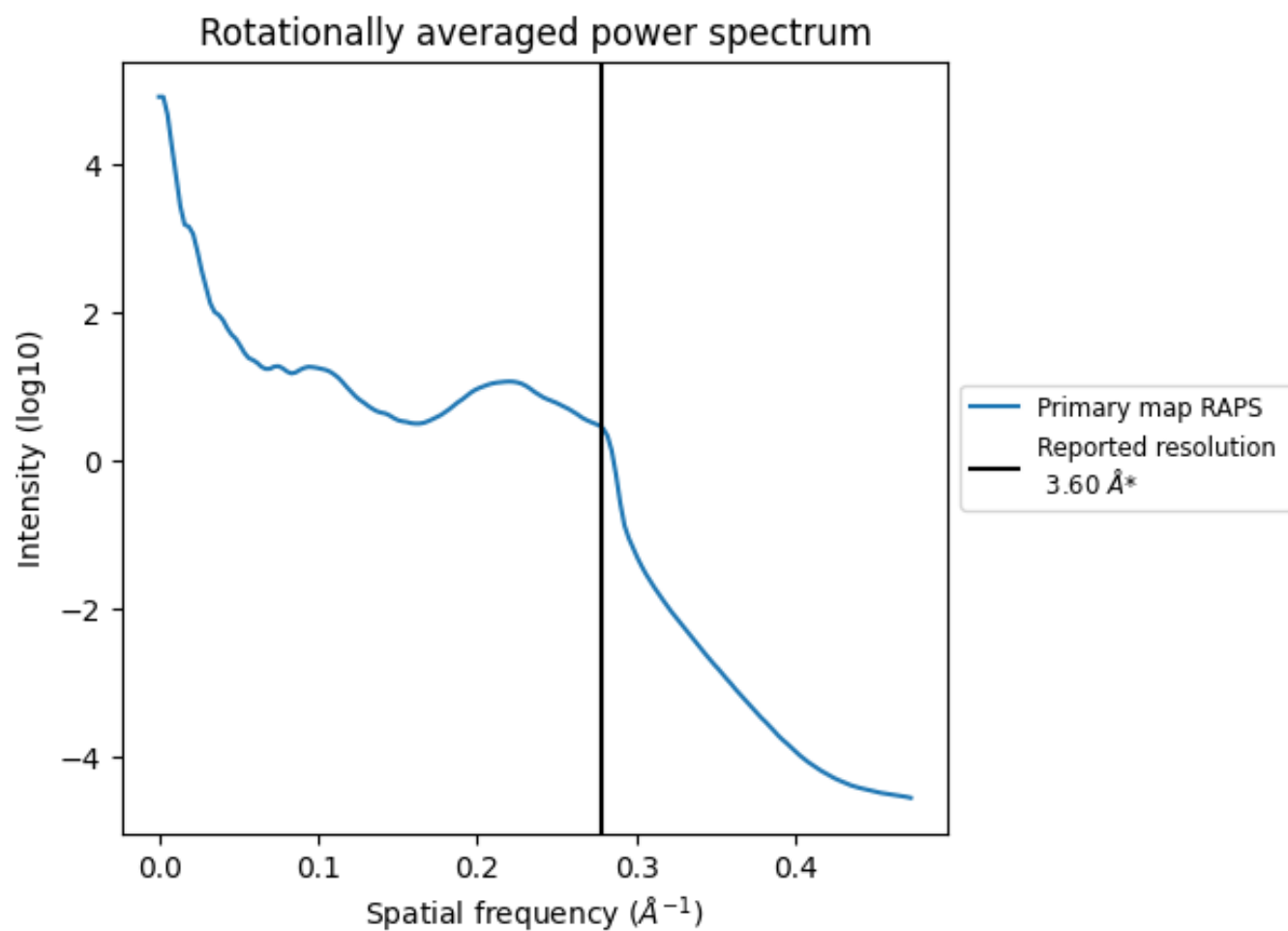
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 103 nm³; this corresponds to an approximate mass of 93 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

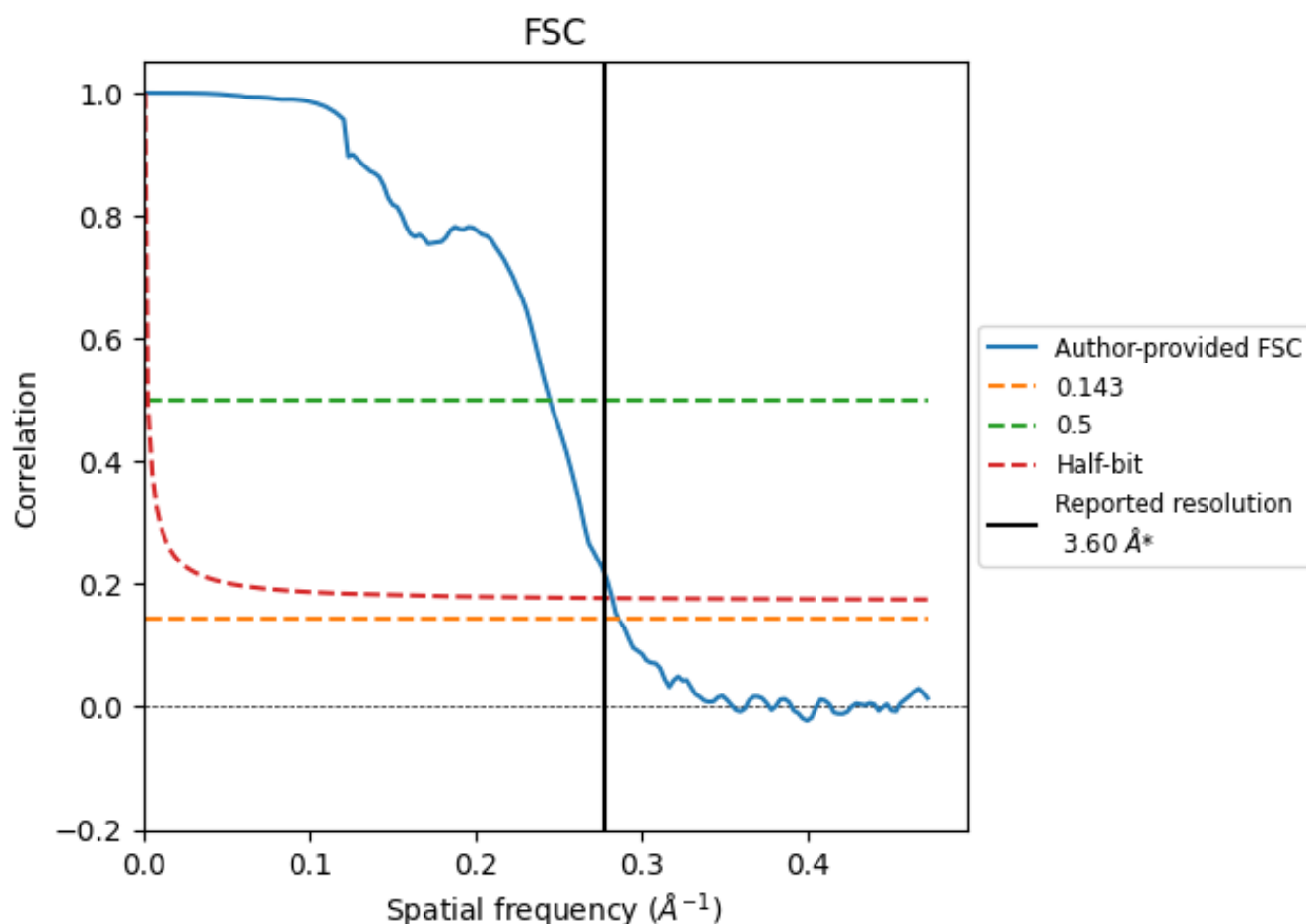


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

8.2 Resolution estimates [i](#)

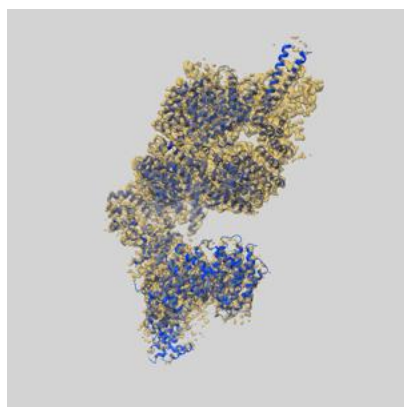
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.49	4.08	3.54
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

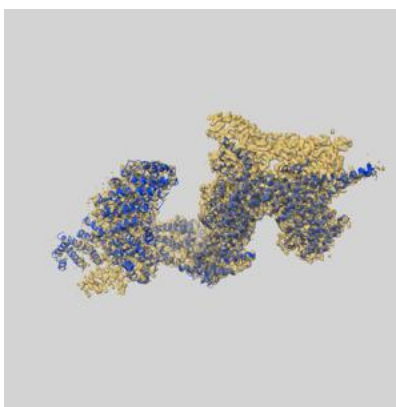
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-10234 and PDB model 6SL1. Per-residue inclusion information can be found in section 3 on page 5.

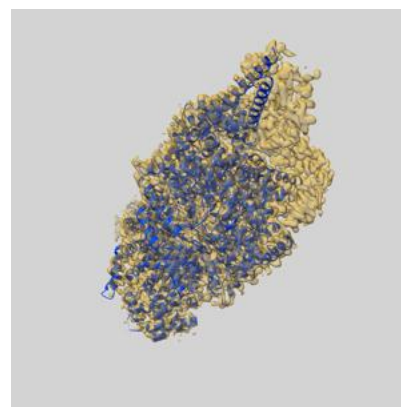
9.1 Map-model overlay [i](#)



X



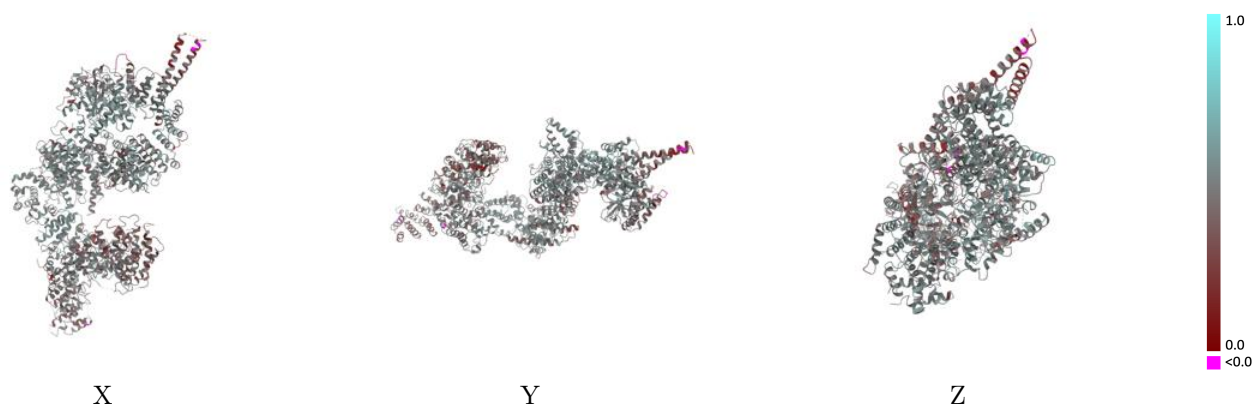
Y



Z

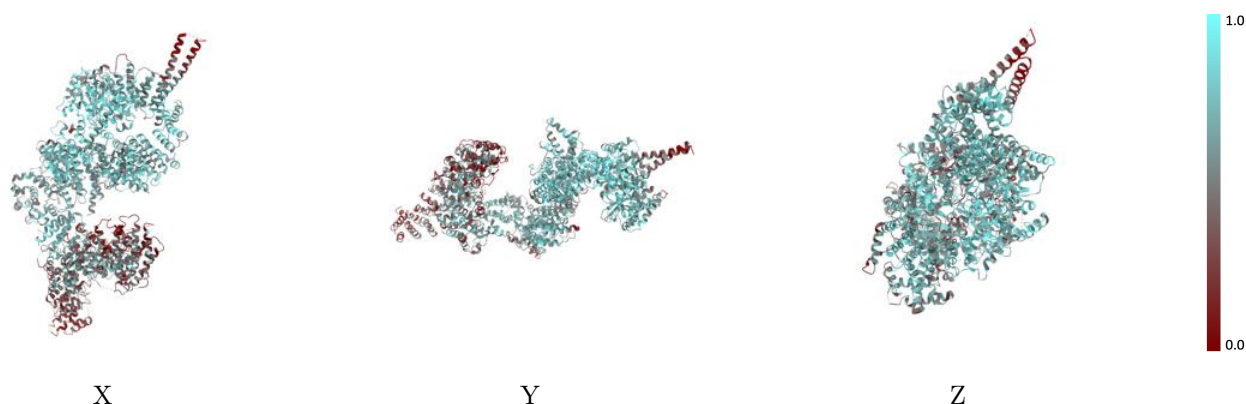
The images above show the 3D surface view of the map at the recommended contour level 0.0118 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



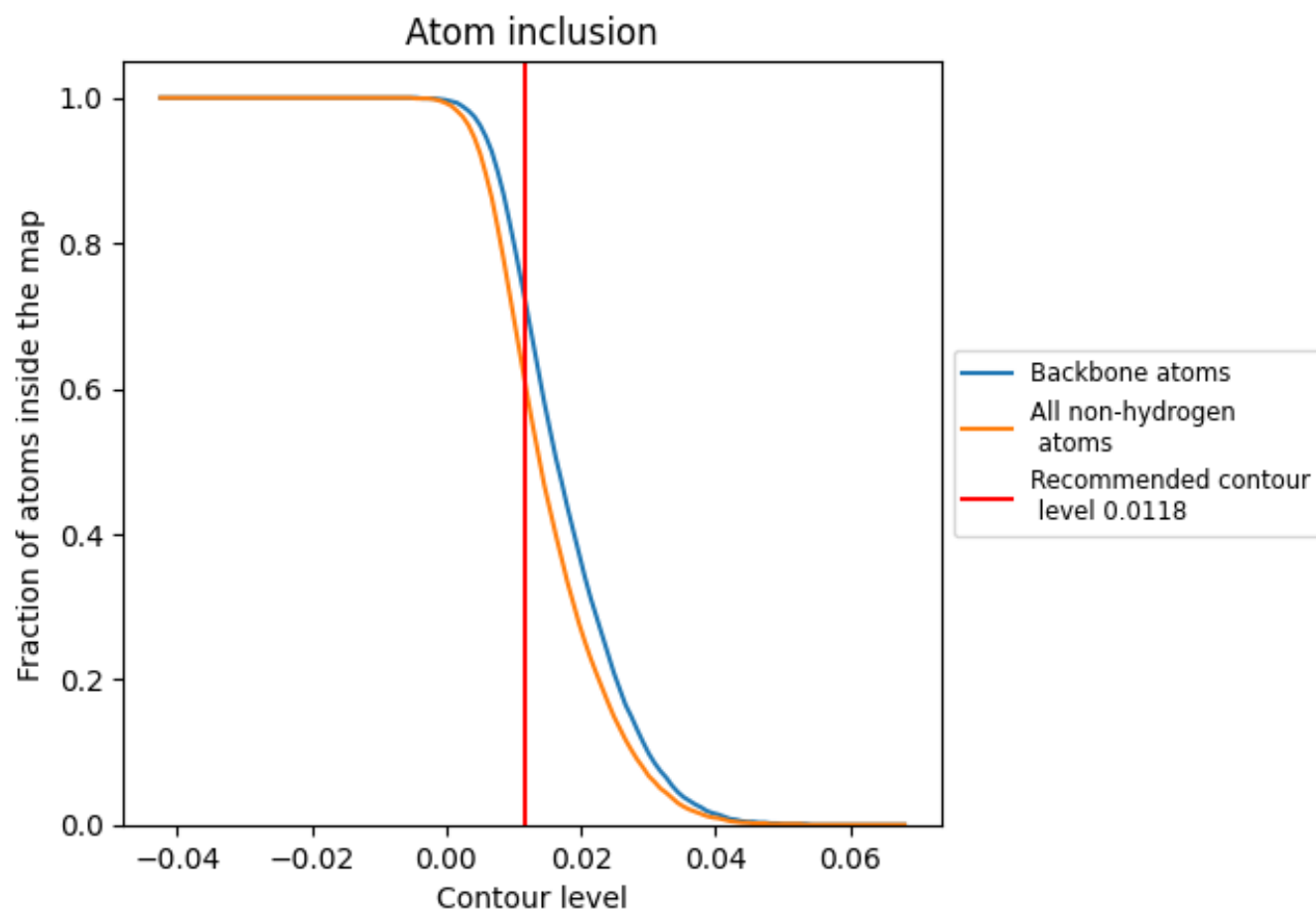
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0118).

9.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 60% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0118) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6040	0.4720
A	0.6040	0.4720

